AROMATICITY IN METALLABORON CLUSTERS

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Metallabenzenes are a class of molecules in which a CH unit in benzene is replaced by a functionalized transition metal atom. While all-boron analogues of aromatic and antiaromatic hydrocarbons are well-known, there have not been any metallaboron analogs using high-resolution photoelectron imaging and quantum chemical calculations. Vibrationally resolved photoelectron spectra have been obtained and compared with theoretical results, determining their structures. Through chemical bonding analyses, we have identified unique aromatic characters in these metallaboron clusters.